Succinic acid, 2,2-dichloroethyl 1-phenylpropyl ester

Inchi: InChI=1S/C15H18Cl2O4/c1-2-12(11-6-4-3-5-7-11)21-15(19)9-8-14(18)20-10-13(16)17/h3
InchiKey: KQUHSOMAGSNQBG-UHFFFAOYSA-N
Formula: C15H18Cl2O4
SMILES: CCC(OC(=O)CCC(=O)OCC(Cl)Cl)c1ccccc1
Mol. weight [g/mol]: 333.21

Physical Properties

Property code	Value	Unit	Source
gf	-308.75	kJ/mol	Joback Method
hf	-648.04	kJ/mol	Joback Method
hfus	35.57	kJ/mol	Joback Method
hvap	77.57	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.808		Crippen Method
mcvol	237.810	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	795.84	K	Joback Method
tc	1011.88	K	Joback Method
tf	459.39	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.14	J/mol×K	795.84	Joback Method
cpg	660.15	J/mol×K	831.85	Joback Method
cpg	672.10	J/mol×K	867.85	Joback Method
cpg	683.03	J/mol×K	903.86	Joback Method
cpg	692.95	J/mol×K	939.87	Joback Method
cpg	701.88	J/mol×K	975.87	Joback Method
cpg	709.85	J/mol×K	1011.88	Joback Method
dvisc	0.0010125	Pa×s	459.39	Joback Method

dvisc	0.0005082	Pa×s	515.47	Joback Method
dvisc	0.0002920	Pa×s	571.54	Joback Method
dvisc	0.0001852	Pa×s	627.62	Joback Method
dvisc	0.0001266	Pa×s	683.69	Joback Method
dvisc	0.0000917	Pa×s	739.77	Joback Method
dvisc	0.0000695	Pa×s	795.84	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389926&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume